(3) Matrix Representation.

Operator X, ket $|\alpha\rangle$, bra $\langle\alpha|$,

.... How can we write them in "numbers"?

(like a wave function, for example.)

$\Rightarrow$ Operator $X \doteq$ Matrix. $\begin{pmatrix} \diagdown \end{pmatrix}$

ket $|\alpha\rangle \doteq$ Column vector. (matrix) $\begin{pmatrix} | \end{pmatrix}$

bra $\langle\alpha| \doteq$ row vector (matrix). $\begin{pmatrix} — \end{pmatrix}$

- Operator

$$X = I \cdot X \cdot I = \sum_i |i\rangle\langle i| \, X \, \sum_j |j\rangle\langle j|$$

$$= \sum_{i,j} |i\rangle \underbrace{\langle i|X|j\rangle}_{\text{a matrix}} \langle j|$$

$$X \doteq \begin{array}{c} \text{col. } j \rightarrow \\ \begin{pmatrix} \langle 1|X|1\rangle & \langle 1|X|2\rangle & \cdots \\ \langle 2|X|1\rangle & \langle 2|X|2\rangle & \cdots \\ & \cdots & \end{pmatrix} \end{array} \quad \downarrow \text{row } i$$

: matrix representation of X in $|i\rangle$-basis.

$\rightarrow$ $Z = XY$: matrix multiplication.

$$\langle i|Z|j\rangle = \langle i|XY|j\rangle = \sum_k \langle i|X|k\rangle\langle k|Y|j\rangle$$

$\rightarrow$ $|\gamma\rangle = X|\alpha\rangle$: matrix-vector multiplication

$$\langle i|\gamma\rangle = \langle i|X|\alpha\rangle$$

$$= \sum_j \langle i|X|j\rangle\langle j|\alpha\rangle$$

X $\qquad \doteq |\alpha\rangle$

$$\Rightarrow \underbrace{\begin{pmatrix} \langle 1|\gamma\rangle \\ \langle 2|\gamma\rangle \\ \vdots \end{pmatrix}}_{\doteq \, |\gamma\rangle \text{ col. vec}} = \begin{pmatrix} \diagdown & & \\ & X_{ij} & \\ & & \diagdown \end{pmatrix} \begin{pmatrix} \langle 1|\alpha\rangle \\ \langle 2|\alpha\rangle \\ \vdots \end{pmatrix}$$

Likewise, bra $\langle \gamma | = \langle \alpha | X$

$$\Rightarrow \quad \underbrace{\langle \gamma | j \rangle}_{\doteq \langle \gamma |} = \sum_i \underbrace{\langle \alpha | i \rangle}_{\doteq \langle \alpha |} \underbrace{\langle i | X | j \rangle}_{\doteq X}$$

$$\Rightarrow \quad \left(\langle \gamma | 1 \rangle, \langle \gamma | 2 \rangle, \cdots \right) = \left(\langle \alpha | 1 \rangle, \langle \alpha | 2 \rangle, \cdots \right) \begin{pmatrix} \ddots & & \\ & X_{ij} & \\ & & \ddots \end{pmatrix}$$

$= \langle 1 | \gamma \rangle^*$ $\quad = \langle 2 | \gamma \rangle^*$ $\qquad\qquad = \langle 1 | \alpha \rangle^*$ $\quad = \langle 2 | \alpha \rangle^*$

" row-vector = row-vec. x Matrix ".

→ inner product. $\langle \beta | \alpha \rangle = \sum_i \langle \beta | i \rangle \langle i | \alpha \rangle$

$$= \left(\langle 1 | \beta \rangle^*, \langle 2 | \beta \rangle^*, \cdots \right) \begin{pmatrix} \langle 1 | \alpha \rangle \\ \langle 2 | \alpha \rangle \\ \vdots \end{pmatrix}$$

as we expect.

→ outer product. $|\beta\rangle\langle\alpha|$: just an operator!

$$|\beta\rangle\langle\alpha| = I \cdot |\beta\rangle\langle\alpha| \cdot I$$

$$= \sum_{ij} |i\rangle \underbrace{\langle i | \beta \rangle \langle \alpha | j \rangle}\langle j |$$

↓

Matrix

$$= \begin{array}{c} \quad i \downarrow \; \longrightarrow j \\ \begin{pmatrix} \langle 1 | \beta \rangle \langle 1 | \alpha \rangle^* & \langle 1 | \beta \rangle \langle 2 | \alpha \rangle^* & \cdots \\ \langle 2 | \beta \rangle \langle 1 | \alpha \rangle^* & \langle 2 | \beta \rangle \langle 2 | \alpha \rangle^* & \cdots \\ & & \ddots \end{pmatrix} \end{array}$$

special case

→ Eigenkets of A as the base ket.

$$A = \sum_{ij} |i\rangle \underbrace{\langle i | A | j \rangle} \langle j |$$

$$\hookrightarrow \langle i | A | j \rangle = a_i \delta_{ij}.$$

$$\Rightarrow \quad A = \sum_i a_i |i\rangle\langle i| = \sum_i a_i \Lambda_i$$

* How to choose the base kets?

- No general Rule … It's usually done by inspection.

- Eigenkets of a physical observable in the H-space that you consider.
  "Known"

ex. In continuum, $\begin{pmatrix} \text{position} \\ \text{momentum} \end{pmatrix}$ operators

"obvious" eigenkets
$|x\rangle, |p\rangle \xrightarrow{\text{def.}}$ wave functions

$\psi(x) = \langle x|\psi\rangle, \ \phi(p) = \langle p|\psi\rangle$

orthogonality

$\langle x'|x\rangle = \delta_{x'x}$, likewise for p.

ex. ~~The~~ Spin-$\frac{1}{2}$ systems.

: $|\uparrow\rangle, |\downarrow\rangle$
  ← Eigenkets of S_z.

ex: Atomic lattice (a single-particle regime)

⟶ atomic basis $|n\rangle$. (single orbital)

⟶ orbital basis (s, p, d, … : "non-orthogonal")

(4) Example: a spin-$\frac{1}{2}$ system.

Eigenstates of S_z-operator: $\begin{pmatrix} |S_z;+\rangle \equiv |\uparrow\rangle \\ |S_z;-\rangle \equiv |\downarrow\rangle \end{pmatrix}$.

Let $|\uparrow\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\quad |\downarrow\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

✓ Completeness: $\mathbb{1} = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|$

$$= \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

eigenvalues of S_z operator in the spin-$\frac{1}{2}$ system.

$$S_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle \quad , \quad S_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle \qquad \text{(SG exp.)}$$

$$\Rightarrow \quad S_z \doteq \begin{pmatrix} \frac{\hbar}{2} & 0 \\ 0 & -\frac{\hbar}{2} \end{pmatrix}.$$

- other operators : $S_+ \equiv \hbar|\uparrow\rangle\langle\downarrow| \quad , \quad S_- = \hbar|-\rangle\langle+|$
  useful.
  $$\doteq \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \doteq \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

1.4 Measurements, observables, and the uncertainty relations

(1) Measurements (on a "pure" state)

Dirac 1958 : " A measurement always causes the system to jump into an eigenstate of the dynamical variable that is being measured ".

$\Rightarrow$ measurement is projective.

ex. measuring an observable associated to an op. "A".

$$A = \sum_i a_i |i\rangle\langle i| \quad , \quad I = \sum_i |i\rangle\langle i|$$

- Before the measurement, the system is at $|\alpha\rangle$.

$$|\alpha\rangle = \sum_a C_i|i\rangle = \sum_i |i\rangle\langle i|\alpha\rangle$$

- Do the measurement : $|\alpha\rangle \xrightarrow{\text{with some probability}} |i\rangle$. !

~~(ex.~~ (exception) (when the system is at an eigenstate !) $|i\rangle \to |i\rangle$ (unchanged)

- probability for jumping into a particular $|i\rangle$

$$= |\langle i|\alpha\rangle|^2 \qquad \parallel \quad \sum_i |\langle i|\alpha\rangle|^2 = 1$$

- expectation value of A (w.r.t. $|\alpha\rangle$)

$$\langle A\rangle = \langle\alpha|A|\alpha\rangle$$

($\doteq$ averaged measured value.)

$$\Rightarrow \quad \langle A\rangle = \sum_{ij} \langle\alpha|i\rangle \underbrace{\langle i|A|j\rangle}_{a_i \delta_{ij}} \langle j|\alpha\rangle$$

$$= \sum_i a_i \quad |\langle i|\alpha\rangle|^2$$

← prob.

↑ measured value

← This is for a "pure" state. ⇐ What we're considering mostly in this course.

: for repeated measurements, all systems are prepared at the same $|\alpha\rangle$.

c.f. "mixed" states (ex. thermal)

- generalization : a density operator. ρ ← We're coming back to this later

pure state : $\rho = |\Psi\rangle\langle\Psi|$

otherwise, it's a mixed state

↳ expectation value $\langle A\rangle = \mathrm{Tr}[\rho A]$

ex. pure state $\rho = |\alpha\rangle\langle\alpha|$

$$\Rightarrow \mathrm{Tr}[\,|\alpha\rangle\langle\alpha| A\,] = \langle\alpha|A|\alpha\rangle$$

(2) spin-$\frac{1}{2}$ system: a review.

- Write everything in $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis.

$\Rightarrow$ $|S_x;\pm\rangle$, $|S_y;\pm\rangle$, S_x, S_y, $\vec{S}^2 = S_x^2+S_y^2+S_z^2$

- $|S_x;\pm\rangle$

Sequential SG exp.

It's the same for $|S_z;-\rangle$ being chosen.

$$\Rightarrow \quad |\langle\uparrow|S_x;\pm\rangle| = |\langle\downarrow|S_x;\pm\rangle| = \frac{1}{\sqrt{2}}$$

Therefore, some phase factor.

$$|S_x;+\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}e^{i\delta_1}|\downarrow\rangle$$

$$|S_x;-\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle - \frac{1}{\sqrt{2}}e^{i\delta_1}|\downarrow\rangle$$

$\rightarrow$ $\langle S_x;+|S_x;-\rangle = 0$

orthogonality condition.

- S_x operator.

: eigenvalues $\frac{\hbar}{2}$, $-\frac{\hbar}{2}$ in $|S_x;+\rangle$, $|S_x;-\rangle$ basis

$$S_x = \frac{\hbar}{2}\Big[\big(|S_x;+\rangle\langle S_x;+|\big) - \big(|S_x;-\rangle\langle S_x;-|\big)\Big]$$

$$= \frac{\hbar}{2}\left[e^{-i\delta_1}|\uparrow\rangle\langle\downarrow| + e^{i\delta_1}|\downarrow\rangle\langle\uparrow|\right]$$

- likewise for S_y

$$|S_y;\pm\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle \pm \frac{1}{\sqrt{2}}e^{i\delta_2}|\downarrow\rangle$$

$$S_y = \frac{\hbar}{2}\left[e^{-i\delta_2}|\uparrow\rangle\langle\downarrow| + e^{i\delta_2}|\downarrow\rangle\langle\uparrow|\right]$$

- How to determine δ_1, δ_2 ?

Rotate the SG axis.

$$\Rightarrow \quad |\langle S_y;\pm|S_x;+\rangle| = |\langle S_y;\pm|S_x;-\rangle| = \frac{1}{\sqrt{2}}$$

$$\Rightarrow \quad \frac{1}{2}\left|1 \pm e^{i(\delta_1-\delta_2)}\right| = \frac{1}{\sqrt{2}}.$$

$$\therefore \quad \delta_1 - \delta_2 = \frac{\pi}{2} \text{ or } -\frac{\pi}{2}$$

Let's just choose δ_1 to make all matrix element of S_z to be **REAL**.

$$\Rightarrow \quad \delta_1 = 0, \quad \delta_2 = \frac{\pi}{2}$$

$\pm\frac{\pi}{2}$ is possible, but $\frac{\pi}{2}$ is correct for Right-handed system.

(Wait for ch. 3)

$$|S_x;\pm\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle \pm \frac{1}{\sqrt{2}}|\downarrow\rangle$$

$$|S_y;\pm\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle \pm \frac{i}{\sqrt{2}}|\downarrow\rangle$$

$$S_x = \frac{\hbar}{2}\left[\,|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\,\right] \rightarrow \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

$$S_y = \frac{\hbar}{2}\left[-i\,|\uparrow\rangle\langle\downarrow| + i\,|\downarrow\rangle\langle\uparrow|\,\right] \rightarrow \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$

- $S_\pm$ operators ; $S_\pm = S_x \pm i S_y$. (raising / lowering operators)

- Commutation, anti-commutation relation.

$$[S_i, S_j] = i\,\varepsilon_{ijk}\hbar S_k, \quad \{S_i, S_j\} = \frac{1}{2}\hbar^2\delta_{ij}$$

* $[A,B] = AB - BA$, $\{A,B\} = AB + BA$

$$\varepsilon_{ijk} = \begin{cases} +1 & (ijk = (123) \text{ and any permutation}) \\ -1 & (ijk = (213) \text{ and any permutation}) \\ 0 & (\text{overlap of indices}) \end{cases}$$

levi-civita.

- $\vec{S}^2 = S_x^2 + S_y^2 + S_z^2 = \underline{\underline{\left(\frac{3}{4}\right)\hbar^2 \cdot \mathbb{1}}}$ ← just compute!

$\Rightarrow [\vec{S}^2, S_i] = 0$. ↑ only for spin-$\frac{1}{2}$.

↑ holds for any spin-S.

(3) Compatible Observables

def.
- Compatible : Commuting! $[A, B] = 0$. (ex. $[\vec{S}^2, S_z]$)
- incompatible : non-commuting! $[A, B] \neq 0$. (ex. $[S_x, S_y]$)

Let's start with Theorem:

If $[A, B] = 0$, the eigenvalues of A are $\underline{\underline{\text{non}}}$degenerate,

‖ eigenkets $|a\rangle \Leftrightarrow a$ (eigenval.)

$\Rightarrow \langle a'' | B | a' \rangle =$ "diagonal"

$\propto \delta_{a'a''}$.

proof.

$\langle a'' | [A, B] | a' \rangle = (a'' - a') \langle a'' | B | a' \rangle = 0$.

$\Rightarrow \langle a'' | B | a' \rangle = 0$ unless $a' = a''$.

☆ Eigenkets diagonalizing A

diagonalizes B as well if $[A, B] = 0$.

"This is also valid even if it (A or B) has degeneracy (eigenvals)."

☆☆☆

$\Rightarrow [A, B] \Rightarrow$ There is a set of

"Simultaneous" eigenkets of A, B"

· Notation $A|a',b'\rangle = a'|a',b'\rangle$ — b' is not relevant

$B|a',b'\rangle = b'|a',b'\rangle$ — a' is not relevant.

← This is an overkill if there is no degeneracy.

But, it's extremely useful when there is degeneracy

ex. $[L^2, L_z] = 0$

→ $\hbar^2 l(l+1)$ ⟶ for l, $m = -l, \cdots l$.

→ $|K\rangle \equiv |l, m\rangle$. ~~specifies~~ characterizes all orbital angular-momentum states.

Thus, it is very important to ~~know~~ find (well, if one can find) ⋯

" a maximal set " of commuting observable.

$[A,B] = [B,C] = [A,C] = \cdots = 0$.

$\Rightarrow |K'\rangle = |a', b', c', \cdots\rangle$

best characterizes the system!

→ of course, it satisfies orthonormality

completeness.

$$\langle K''|K'\rangle = \delta_{a''a'}\delta_{b''b'}\cdots$$

$$\sum_{K'} |K'\rangle\langle K'| = \sum_{a',b',c',\cdots} |a',b',c',\cdots\rangle\langle a',b',c',\cdots| = 1.$$